Tris(2-butoxyethyl) phosphate
78-51-3 | DTXSID5021758

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.71e-05 mmHg

Global applicability domain: Outside

Local applicability domain index: 2.37e-01

Confidence level: 5.96e-01

Nearest Neighbors from the Training Set

Image not found
Chloroacetaldehyde
Measured: 2.60e-04
Predicted: 81.8

Image not found
2,3-Dichlorobutane
Measured: 1.40e-05
Predicted: 18.3

Image not found
Fenchol
Measured: 9.80e-06
Predicted: 6.35e-02

Image not found
(1R)-endo-(+)-Fenchyl alcohol
Measured: 9.80e-06
Predicted: 6.35e-02

Image not found
Indanofan
Measured: 2.30e-07
Predicted: 3.60e-08

Image not found
Flubenzimine
Measured: 8.00e-05
Predicted: 2.90e-06